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Features of Indoor Human Surface Chemical Reaction under Displacement Ventilation

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Abstract

Ozone reactions with human surfaces (skin, hair, and clothing) are an important source of volatile organic compounds in the indoor air, which play an important role in indoor air quality and building occupant health. It's the purpose of this study to obtain the characteristics of air change rate (ACH) and reactants concentration impacting human surface chemical reaction, which is very necessary and meaningful for guiding how to improve indoor air quality (IAQ). Theoretical model describing indoor human surface chemical reaction between O3 and Squalene, heat and mass transfer was established and verified. Meanwhile, three kinds of factors were taken into account and their influence on human surface chemical reaction under displacement ventilation was analyzed for typical building space. The results show that the rising of ACH is benefit for reducing the exposure concentration of product (secondary pollutant) under displacement ventilation. Moreover, lowering ozone concentration in supplied air and squalene concentration in human surface is very meaningful for improving IAQ.

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Keywords: Indoor air quality; Human surface; Chemical reaction; Displacement ventilation

1. Introduction

Chemical reaction occurring on human surfaces (skin, hair, and clothing) can alter the concentrations of both reactants and products, the latter have more irritant and produce obvious impact on IAQ and human health. Some previous studies had focused on ozone (O_3) induced related indoor chemical reactions. Wisthaler (2005) used proton-transfer-reaction mass spectrometry (PTR−MS) to examine the products formed when ozone reacted with the materials

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in a simulated aircraft cabin, including a loaded high-efficiency particulate air (HEPA) filter in the return air system [1]. Destaillats (2006) investigated secondary air pollutants formed from reactions between constituents of household products and ozone [2]. Pandrangi (2008) determined the cumulative ozone uptake, the ozone reaction probability and product yields of volatile aldehydes and ketones for human scalp hair [3]. Wisthaler (2010) used proton transfer reaction-mass spectrometry (PTR-MS) for direct air analyses of volatile products resulting from the reactions of ozone with human skin lipids [4]. Nazaroff and Weschler (2010) found ozone reacted rapidly with skin lipids present on the exposed skin, hair and clothing of the cabin occupants [5]. Rai (2014) established empirical models for computing the emissions of several major volatile organic compounds, including acetone, 4-oxopentanal, nonanal, and decanal, from ozone reactions with human-worn clothing [6]. It can be found from the above studies that there's lacking relevant research on microscopic features of human surfaces chemical reaction under the influence of typical factors, which is to be determined in this present study.

Nomenclature

S	the source term
U	the air velocity
ϕ	the common variable
ρ	the air density
Γ	the diffusion coefficient
γ	the mass accommodation coefficient
$\langle v_T \rangle$	the Boltzmann velocity for ozone
Δy_1	the distance to the center of the first computational cell

2. Methods

2.1. Theoretical model

Mass, momentum, turbulence and energy conservation of indoor air were taken into consideration under ventilation conditions and human surface chemical reaction occurring. As there was obvious difference between the Reynolds number (Re) in bulk air and that of air layer near human surface, the turbulence of air flow, heat and mass transfer through human surface were described by the Low-Re k-ε model and the buoyancy effects. The corresponding theoretical model of indoor air is as the following equation:

$$\frac{\partial}{\partial t}(\rho\phi) + \mathrm{div}(\rho U \phi) = \mathrm{div}(\Gamma_\phi \mathrm{grad}\phi) + S_\phi \tag{1}$$

where ϕ is the common variable; ρ is air density; U is the air velocity; Γ_ϕ is the diffusion coefficient; S_ϕ is the source term. As there was only human surface chemical reaction, the source term equaled to zero.

Squalene was the most abundant unsaturated compound in human sebum. The main human surface chemical reaction was occurring between ozone (O_3) and squalene ($C_{30}H_{50}$), shown in Fig. 1, which could be seen as bimolecular chemical reaction and depicted as following:

$$\frac{d[\mathrm{P}]}{dt} = -\frac{d[\mathrm{O_3}]}{dt} = -\frac{d[\mathrm{C_{30}H_{50}}]}{dt} = k[\mathrm{O_3}][\mathrm{C_{30}H_{50}}] \tag{2}$$

This kind of reaction may produce acetone, 6-methyl-5-hepten-2-one, 4-oxopentanal, et al. For the purpose of this study, it was assumed that this kind of reaction produced a single hypothetical product. In addition, according to molecular theory, the ozone surface deposition of local concentration close to the human surface, the flux at the surface was given as the following:

$$J = -\frac{\gamma \cdot \frac{<v_T>}{4}}{1 + \gamma \cdot \frac{<v_T>}{4} \cdot \frac{\Delta y_1}{D_1}} \cdot C_1 \Big|_{y=\Delta y_1} \tag{3}$$

where γ is the mass accommodation coefficient; $<v_T>$ is the Boltzmann velocity for ozone; Δy_1 is the distance to the center of the first computational cell.

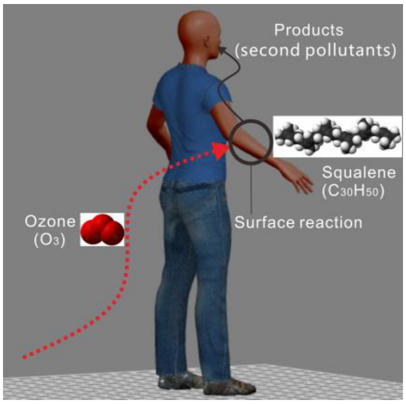

Fig. 1. Human surface chemical reaction occurring between by ozone and squalene.

2.2. Verification of theoretical model

Indoor environment experiment system built in Sichuan University was used for verifying the above theoretical model. The indoor space modeled by the system had dimensions of 1.5 m (width) × 2.5 m (length) × 2.3 m (height) and equipped with displacement ventilation, shown in Fig. 2(a). As vector determined the change of the scalar, the velocity of the y direction at 0.2 meters front and back of manikin and 1.5 meters above the ground portion were measured by KANOMAX 6243 under different air change rates (ACH). In order to obtain accurate measured results and reduce error, the velocity on the y direction for each ACH was tested by five times. Then, the mean value of the velocity on the y direction can be obtained.

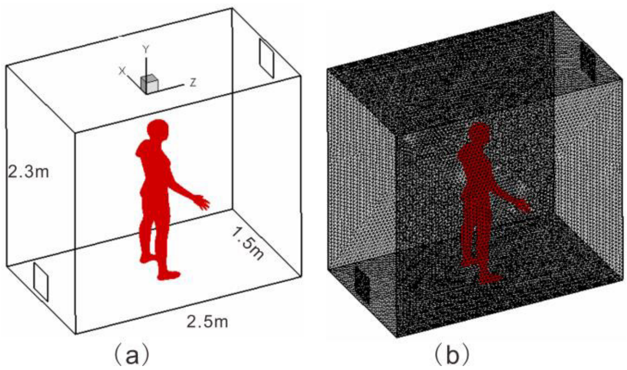

Fig. 2. Indoor space selected for simulation: (a) geometry size; (b) grid division.

The finite volume method was utilized to discretize equations of this present model in the simulating region. Evaluation of the advection terms of Navier-Stokes equations, turbulent transport, mass and energy equations was achieved by the QUICK scheme. The central differencing algorithm was used for two-order implicit scheme. The SIMPLEC algorithm was applied to the pressure-velocity coupling. Grid-independent solution was tested by using three levels of non-structured grid sizes, the quantity of final mesh used in this simulation was 1900923, which was demonstrated in Fig. 2(b). The comparison of recorded data to simulated values for the velocity of the y direction under 52 W/m^2 of the manikin heat flux was given in Fig. 3. The percentages of error in simulation results were less than 5%, which showed their well consistency and indicated that the present model can simulate momentum and heat transfer of indoor air accurately.

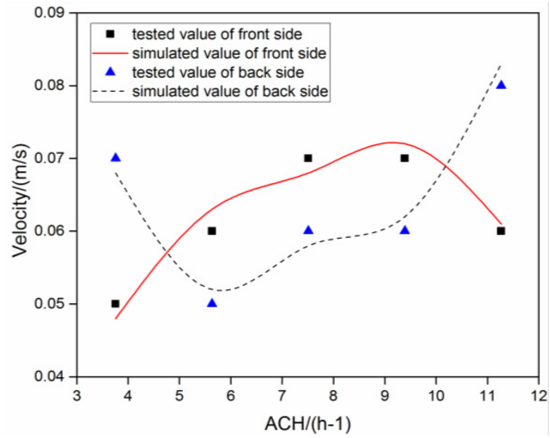

Fig. 3. Comparison between measured data and simulated values of the y direction velocity.

3. Results

When binary diffusion coefficients of ozone and product (secondary pollutant) are 1.82×10^{-5} m^2/s and 1.049×10^{-5} m^2/s, respectively, deposition velocity of ozone is 0.0018 m/s, reaction rate is 0.001098 /(ppb.h), ozone and product (second pollutant) distributions in the above indoor space with displacement ventilation are obtained for different ACH, ozone concentration of supplied air, squalene concentration on human surface.

3.1. Impact of ACH

Firstly, change of ACH (n) can induce effect of human thermal plume and bodyforce to vary, further, lead air temperature having different distribution, seen Fig. 4. It can be found that the increase of ACH may lower the effect of human thermal plume and bodyforce. Moreover, the temperature stratification becomes not obvious gradually.

Secondly, when ozone concentration in supplied air and squalene concentration in human surface keep 40 ppb and 27.29 ppb, respectively, as indoor ozone is derived from supplied air, the rise of ACH can cause the ozone amount entering into indoor space per unit time to increase, and then the exposure concentration of ozone nearby human body has obvious ascending, shown in Fig. 5.

Meanwhile, when the ACH rises from 5 h^{-1} to 10 h^{-1} and then to 15 h^{-1}, the exposure concentration of ozone increases by 38.1% and 17.2%, respectively. In addition, the ascending of ozone exposure concentration may enhance the human surface chemical reaction between ozone and squalene. Accordingly, more reaction product should be produced theoretically. However, the increasing of ACH can make the residence time of reactants and product in indoor space to decrease. Moreover, dilution effect of ventilation air flow may be enhanced as a result of the rise of ACH. Therefore, the exposure concentration of product decreases by 28.0% and 22.2%, correspondingly, seen in Fig. 6, when the ACH rises from 5 h^{-1} to 10 h^{-1} and then to 15 h^{-1}.

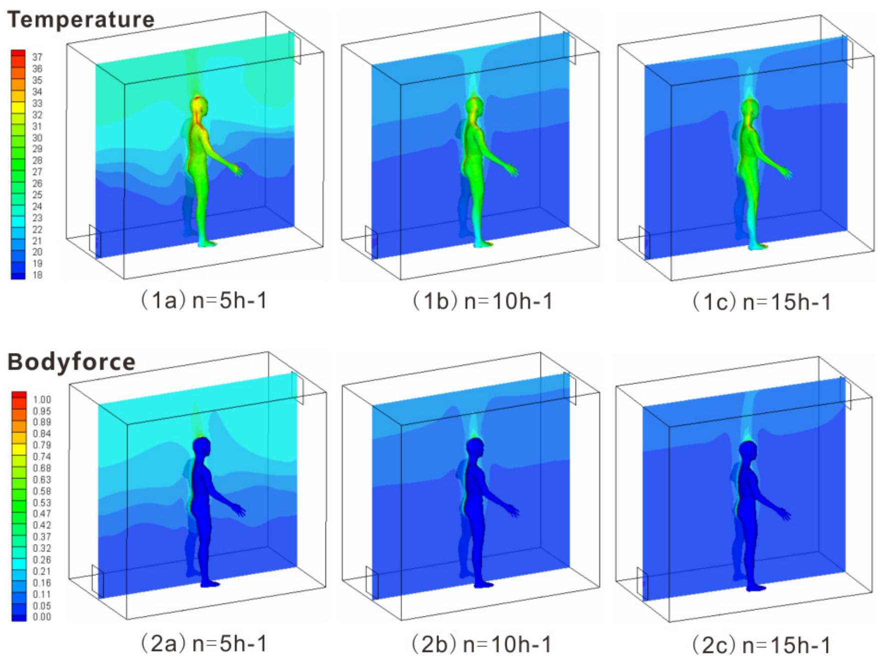

Fig. 4. Distribution of indoor air and human body surface temperature and bodyforce.

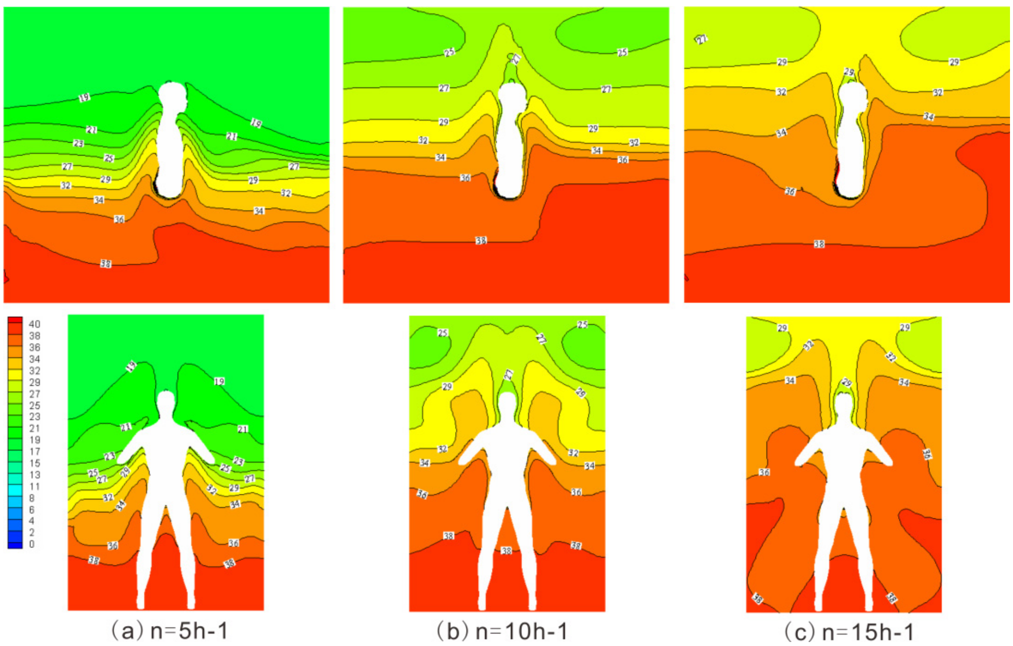

Fig. 5. Indoor ozone concentration distribution under different ACH (ppb).

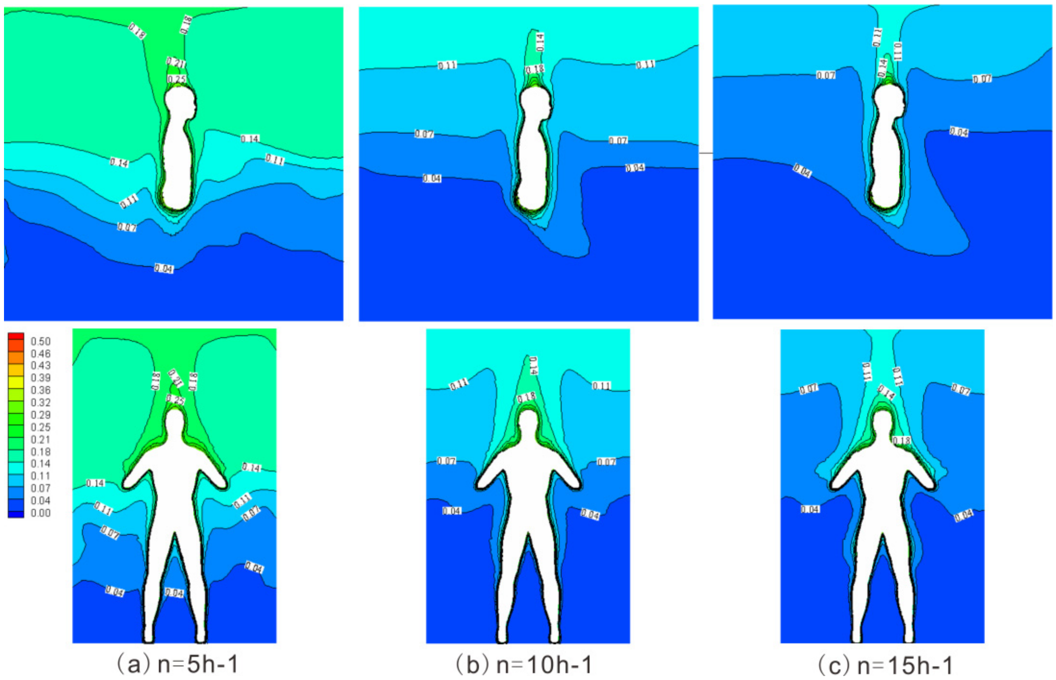

Fig. 6. Indoor product concentration distribution under different ACH (ppb).

3.2. Impact of ozone concentration in supplied air

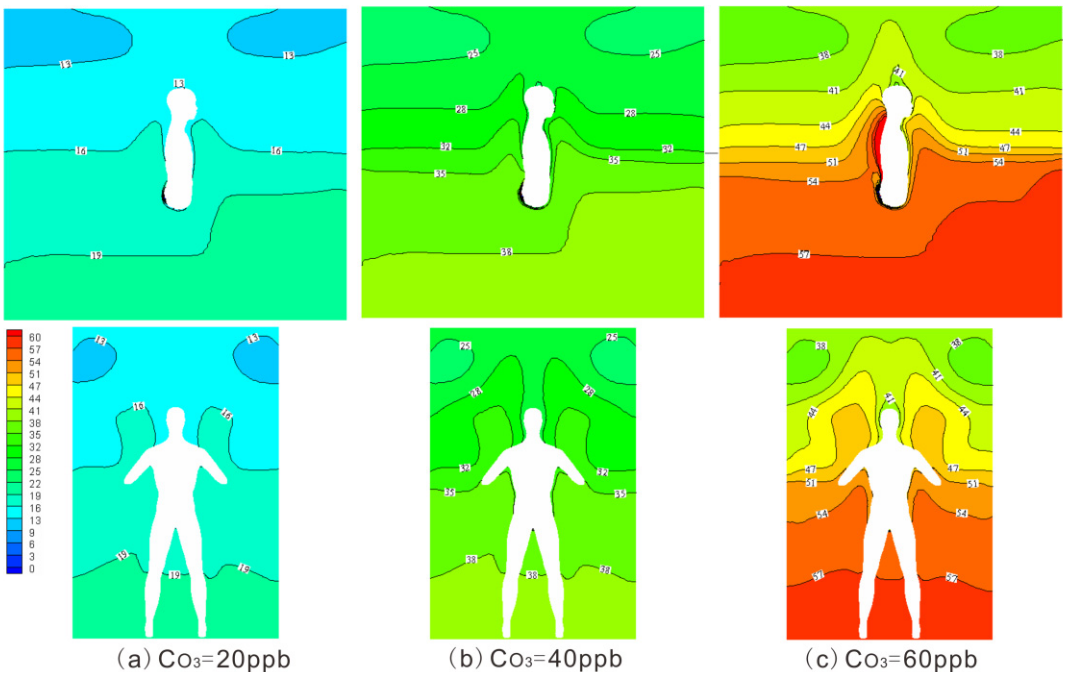

Fig. 7. Indoor ozone concentration distribution under different C_{O3} (ppb).

For the ACH of 10 h^{-1} and squalene concentration of 27.29 ppb, increasing of ozone concentration in supplied air (C_{O3}) may lead the exposure concentration of ozone nearby human body to rise, shown in Fig. 7, which may enhance the human surface chemical reaction between ozone and squalene. Accordingly, as the C_{O3} rises from 20 ppb to 40 ppb and then to 60 ppb, the exposure concentration of product ascends by 54.5% and 35.3%, correspondingly, seen in Fig. 8.

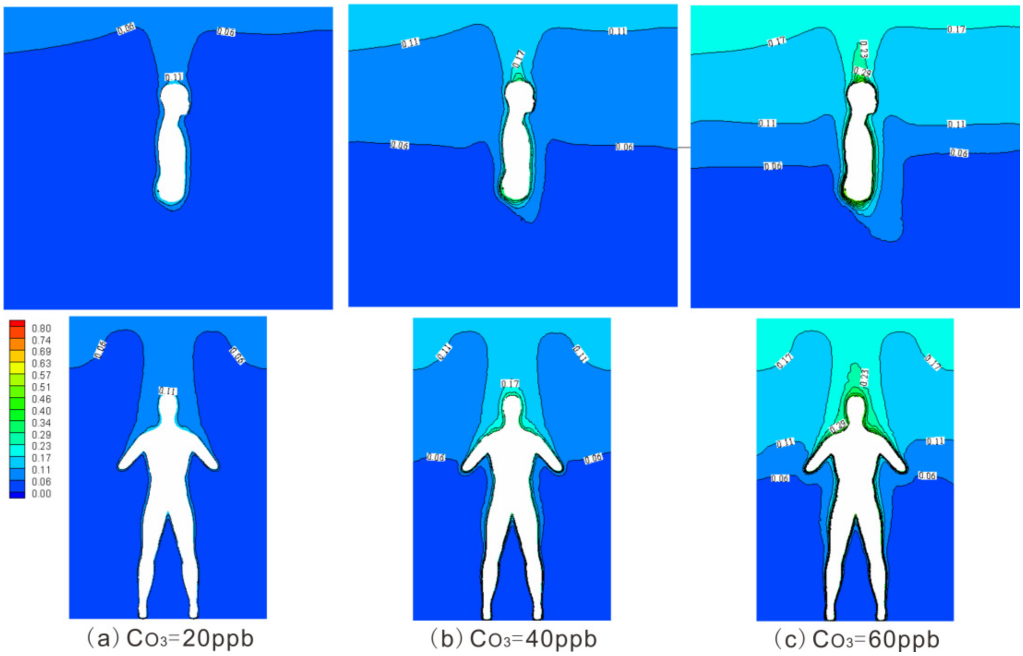

Fig. 8. Indoor product concentration distribution under different C_{O3} (ppb).

3.3. Impact of squalene concentration in human surface

As to the ACH of 10 h^{-1} and ozone concentration in supplied air of 40 ppb, rise of squalene concentration in human surface (C_s) merely induces slight influence on ozone distribution, seen in Fig. 9. However, obvious ascending of product exposure concentration emerges as a result of rise of squalene concentration. When the C_s rises from 13.64 ppb to 27.29 ppb and then to 40.93 ppb, the exposure concentration of product increases by 63.6% and 38.9%, respectively, shown in Fig. 10.

4. Discussion

According to the above results, it can be found that there exist dual impacts of the ACH on indoor chemical reaction. The change of ACH may lead the indoor ozone concentration and product concentration, their residence time to vary along the opposite direction. Namely, rising of ACH may cause the indoor ozone to ascend as it is derived from the supplied air. However, the product concentration and the zone and product residence time can be reduced as a result of rising of ACH. Even so, the rise of ACH is benefit for decreasing the exposure concentration of product (secondary pollutant) under displacement ventilation.

In addition, the ascending of ozone concentration in supplied air and squalene concentration in human surface can induce the human surface chemical reaction to be enhanced, especially for the latter. Therefore, high efficient and clean ventilation system is very needed for controlling this kind of secondary pollution and improving indoor air quality. Moreover, clean hair, skin and cloth of human is one fundamental method for reducing the reactant and also benefit for the above point.

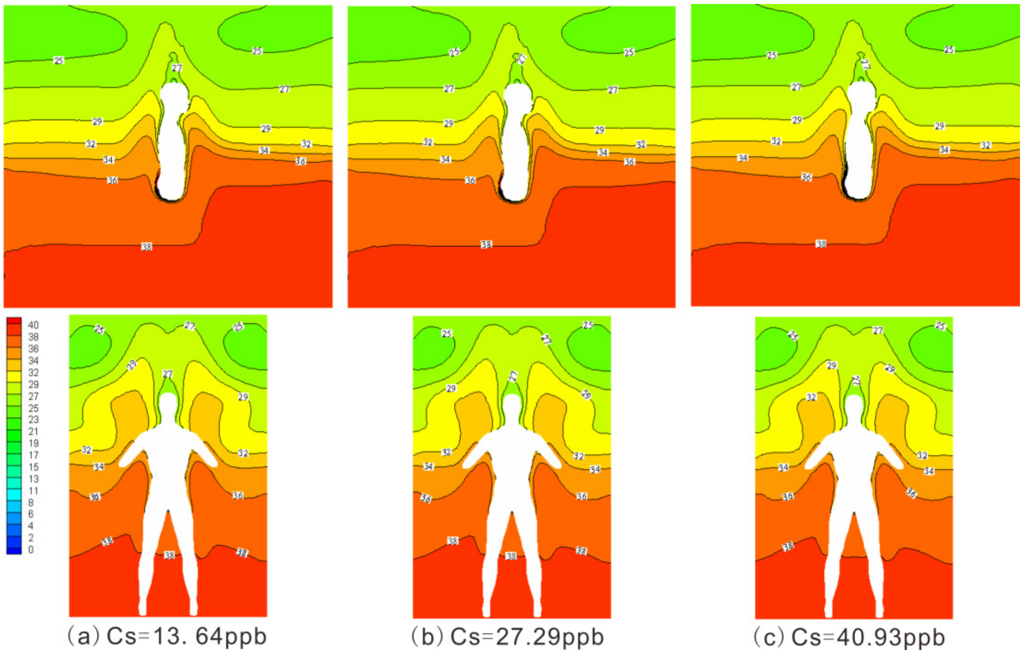

Fig. 9. Indoor ozone concentration distribution under different C_s (ppb).

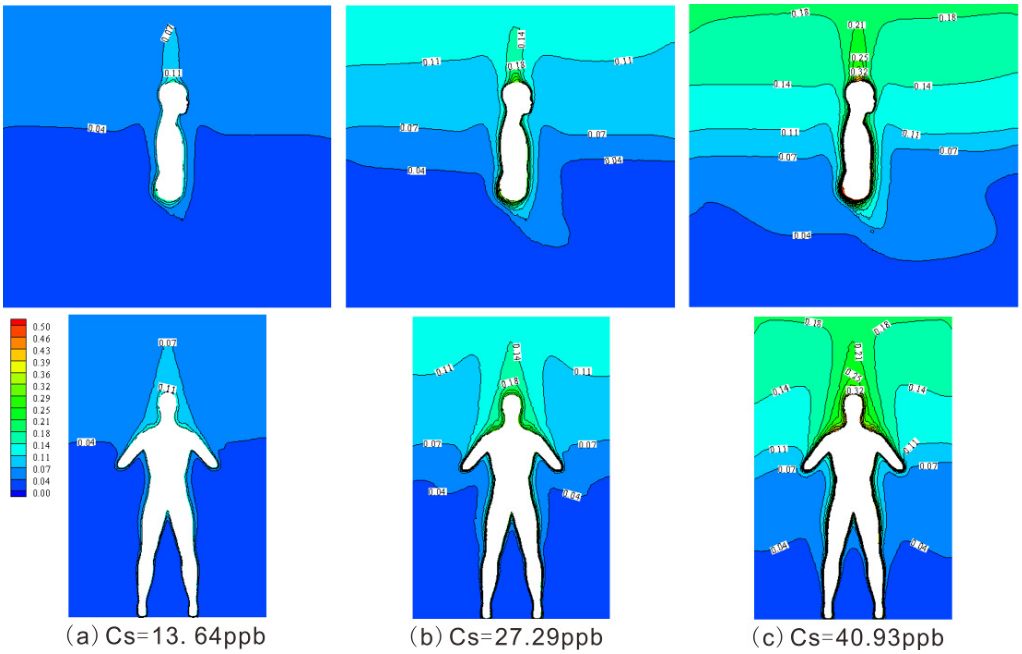

Fig. 10. Indoor product concentration distribution under different C_s (ppb).

5. Conclusions

As to the indoor human surface chemical reaction between ozone and squalene, theoretical model describing this kind of reaction, heat and mass transfer was established and verified. Meanwhile, the influence of air change rate (ACH) and reactants concentration on human surface chemical reaction was analyzed for typical building space with displacement ventilation. The research results indicate that the increasing of ACH is conducive to reduce the exposure concentration of product (secondary pollutant) and improve IAQ under displacement ventilation. Lowering ozone concentration in supplied air and squalene concentration in human surface is very necessary for controlling indoor secondary pollution.

Acknowledgements

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